Overview of Combustion Research Activities at the University of Utah

Programs, Capabilities and Facilities in the

Department of Chemical and Fuels Engineering

at the University of Utah

DOE Combustion Technology

University Alliance Workshop

August 4-5, 2003

Combustion Research Personnel at the University of Utah

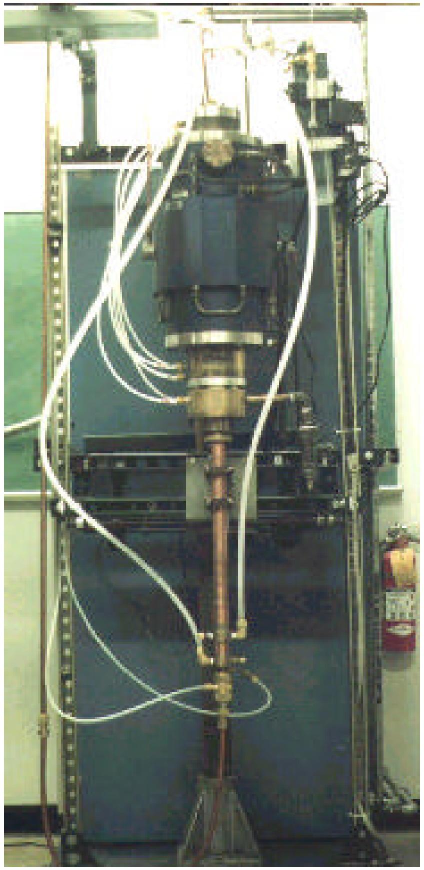
- Faculty/Research Staff
  - Eric Eddings, JoAnn Lighty, Ron Pugmire, David Pershing, Rajesh Rawat, Adel Sarofim, Geoff Silcox, Philip Smith, Jennifer Spinti, Sheshadri Kumar, Angela Violi, Kevin Whitty
- Professional Staff
  - 10 engineers, post-docs and admin
- Current Students
  - 18 Ph.D., 4 M.S., 9 B.S.

Research Emphasis

- Research activities encompass fundamental computation and experimental efforts, through pilot-scale validation, to computational simulation of full-scale processes
- Our research efforts can be divided into the following areas:
  - Mechanism Identification (Experimental/Computational)
  - Mechanism Development
  - Process Development and Verification
  - Process Simulation

Mechanism Identification - Experimental

Solid Fuel Drop-Tube Furnace

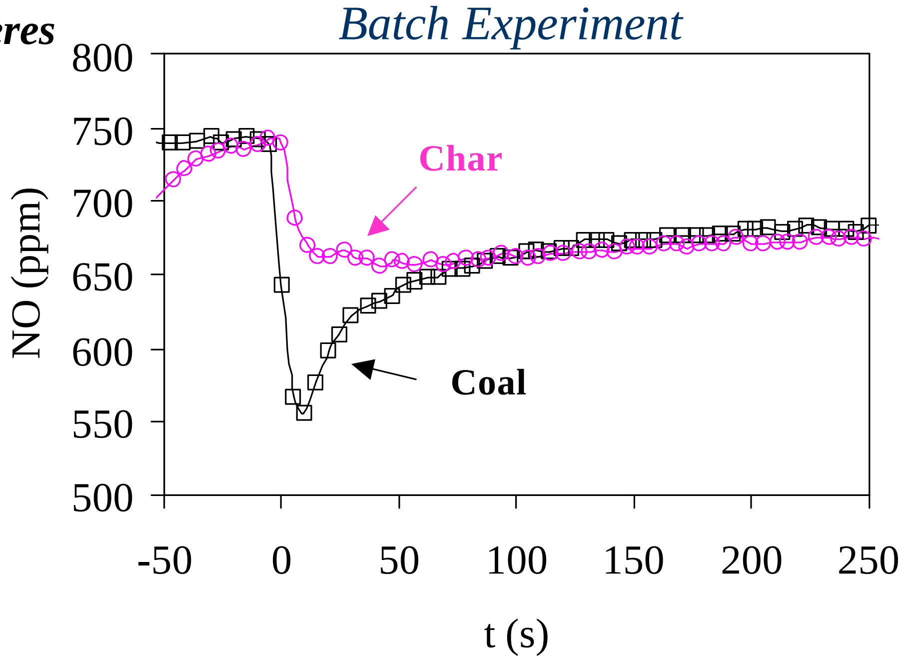


<u>Entrained Flow Reactors for High Temperature Coal, Coke and Biomass Reaction Kinetics:</u>

- electrically heated – maximum of 2300 K

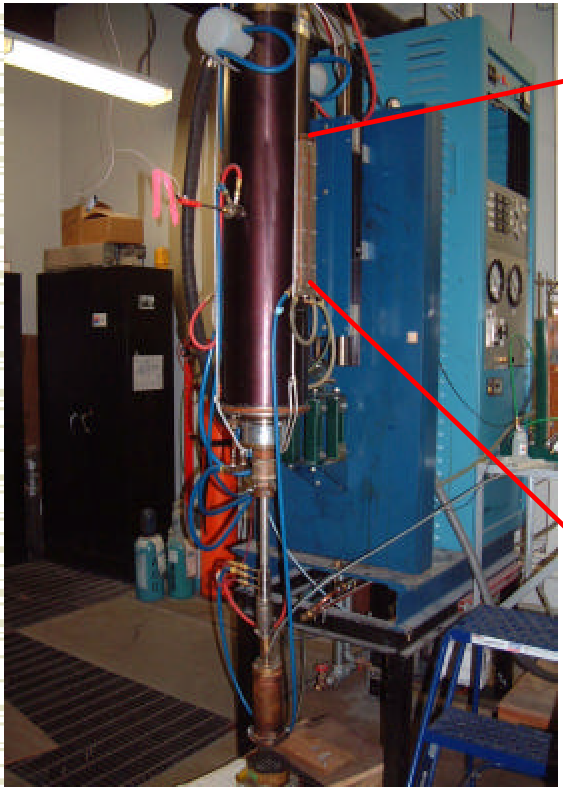
- reaction times to 1 sec

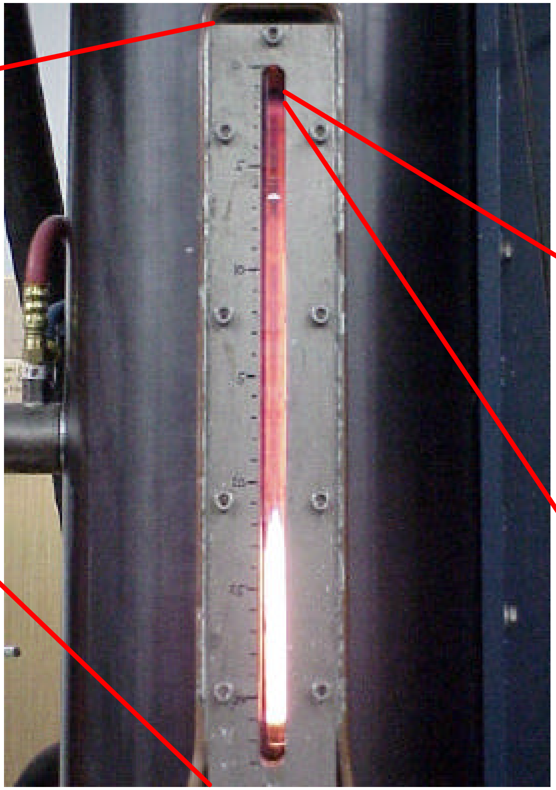
- range of atmospheres



Reburning with char vs. coal in a 750 ppm NO/He stream. Solids are injected at time=0. Temperature = 1273 K.

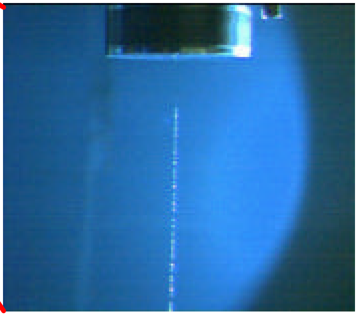
Liquid Fuel Drop-Tube Furnace





Laminar Flow Reactor for High Temperature Liquid Fuel Combustion Studies:

- ***electrically heated – maximum of 1700 K***
- ***reaction times to 1 sec***
- ***range of atmospheres***
- ***optical access***

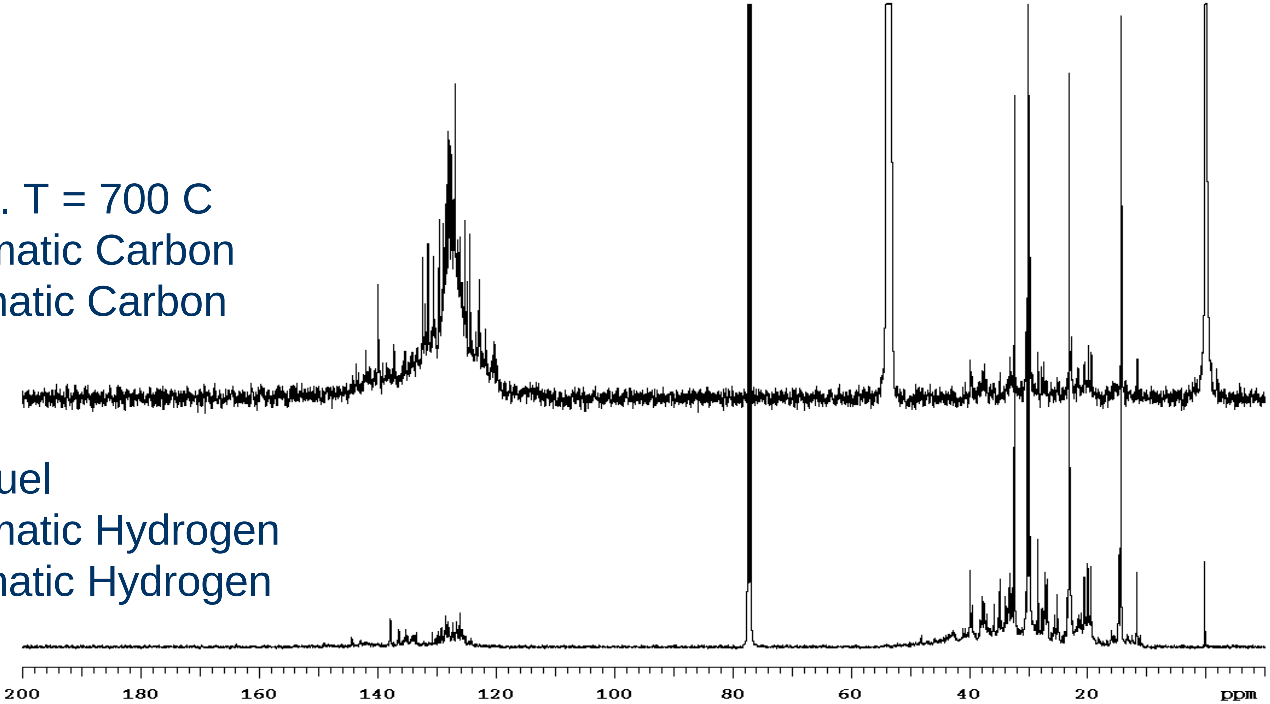


A monodisperse droplet stream is injected into a hot, co-flow air stream, producing a laminar diffusion flame.

^{13}C NMR Spectra of Soot Extract vs. Spectra of Pure Liquid Fuel (Jet- A)

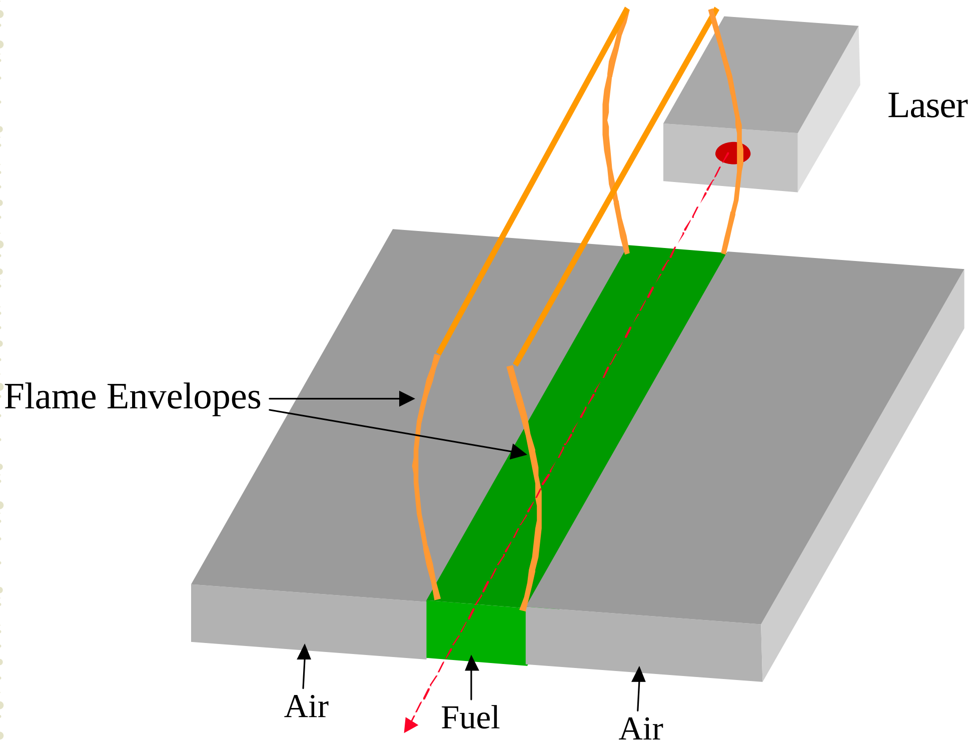
Soot Extract. T = 700 C
76.6 % Aromatic Carbon
23.4 % Aliphatic Carbon

Pure liquid fuel
10.6 % Aromatic Hydrogen
89.4 % Aliphatic Hydrogen

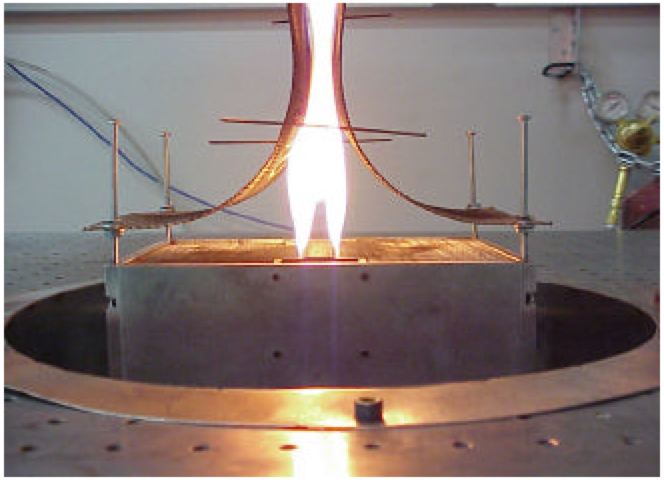


Most of the aliphatic carbon becomes aromatic carbon when the Jet Fuel is burned at 700 C.

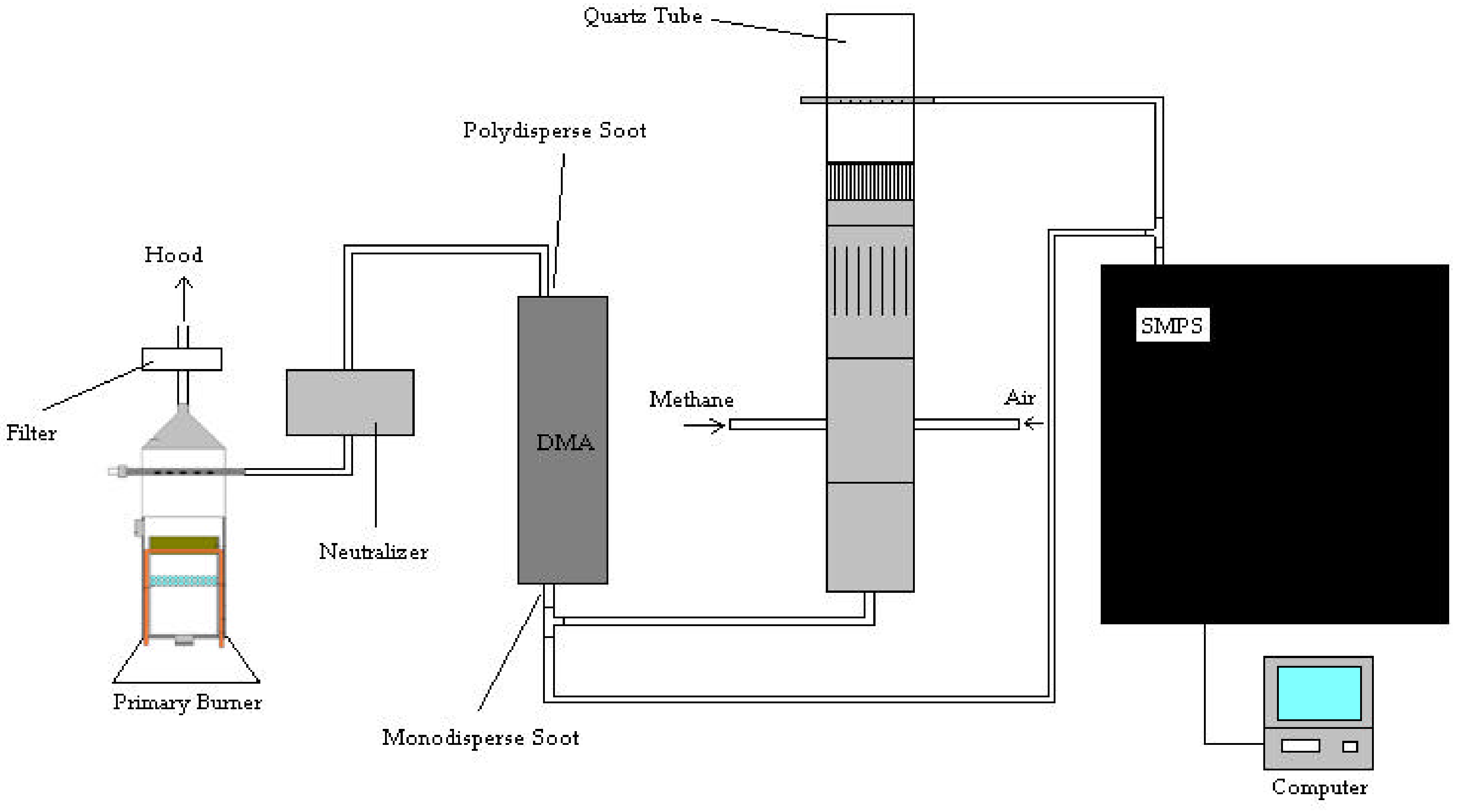
2-D Laminar Slot Burner



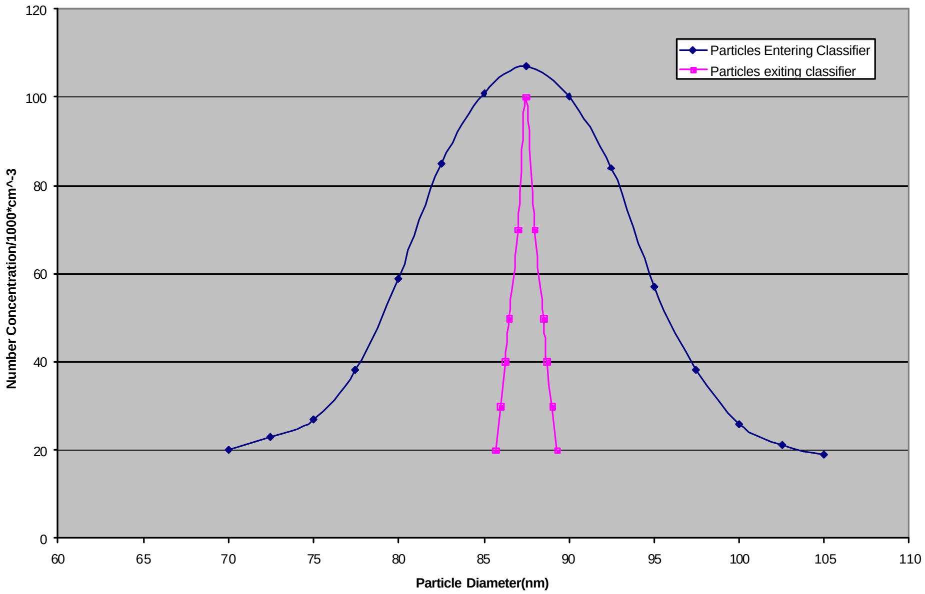
__Laminar Slot Burner facility:__
-Diffusion flame studies
-Laser-based diagnostics
-Project of 2-D flame over distance to provide for greater absorption for determining species concentration and temperature



Two-Stage Soot Oxidation Experiment



Two-Stage Soot Oxidation Experiment



Size Selection in Intermediate DMA Classifier

Combination of Two Premixed Burners:

-Carbon particulate created in first burner under wide variety of conditions

-Particle effluent from first pre-mixed burner sent through DMA Classifier

- Narrow-size distribution then sent through second burner for study of oxidation kinetics

-Operating conditions of second burner can be varied independent of first burner

-Use of electrospray atomization for heavy liquid fuels

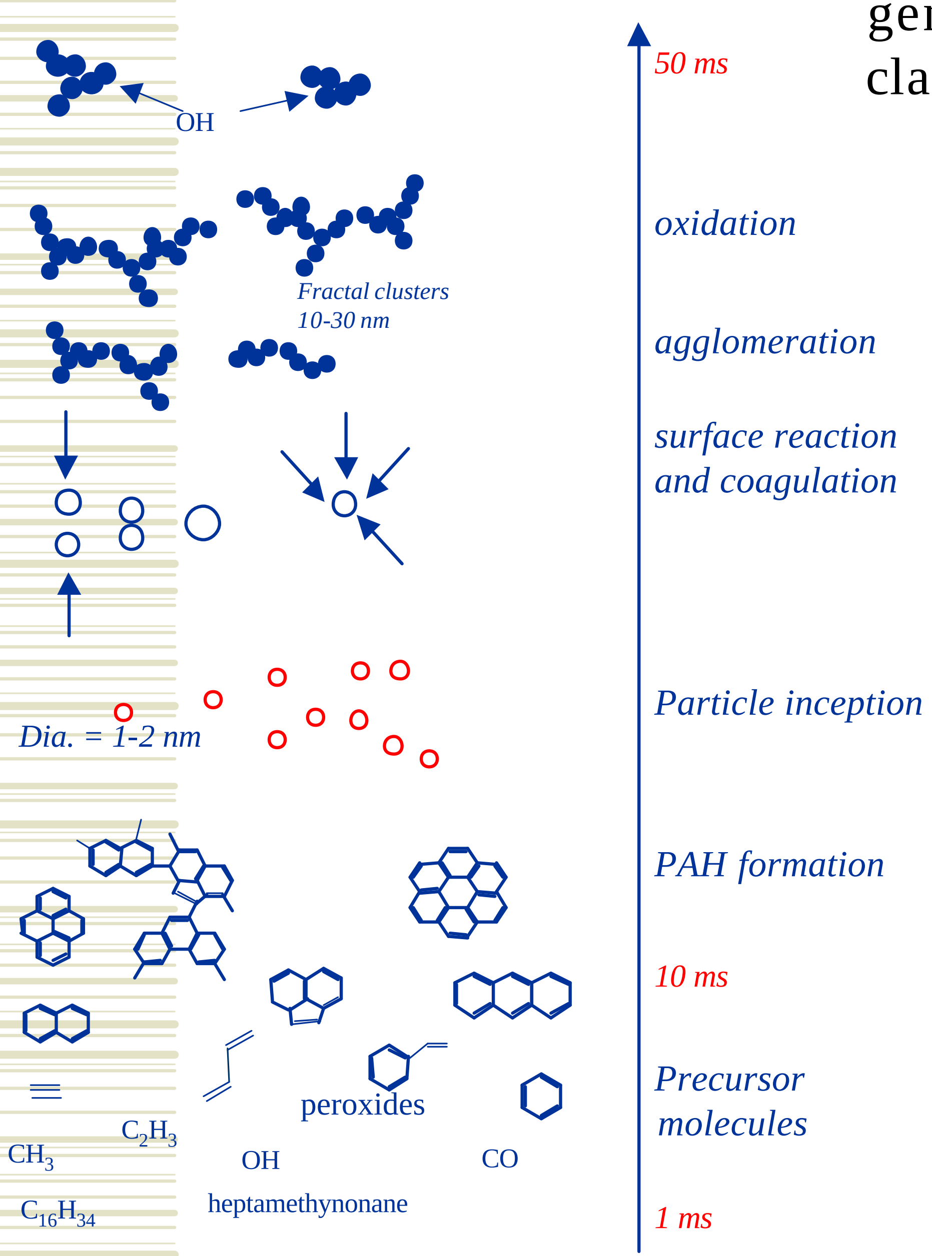
Mechanism Identification - Computational

Quantum Chemistry Calculations

- Various ab initio techniques are used to provide:
  - Information on thermodynamic favorability of certain reaction pathways
  - Rate information for difficult to measure reaction rates
  - Structural information
  - Current applications include:
    - Species involved in NOx chemistry
    - Species involved in heavy HC fuel chemistry and soot particle formation

Development and **validation** of first generation of soot model based on classical and modern tools including:

- ab initio calculations
- fundamental chemical and physical models
- comparison with literature data

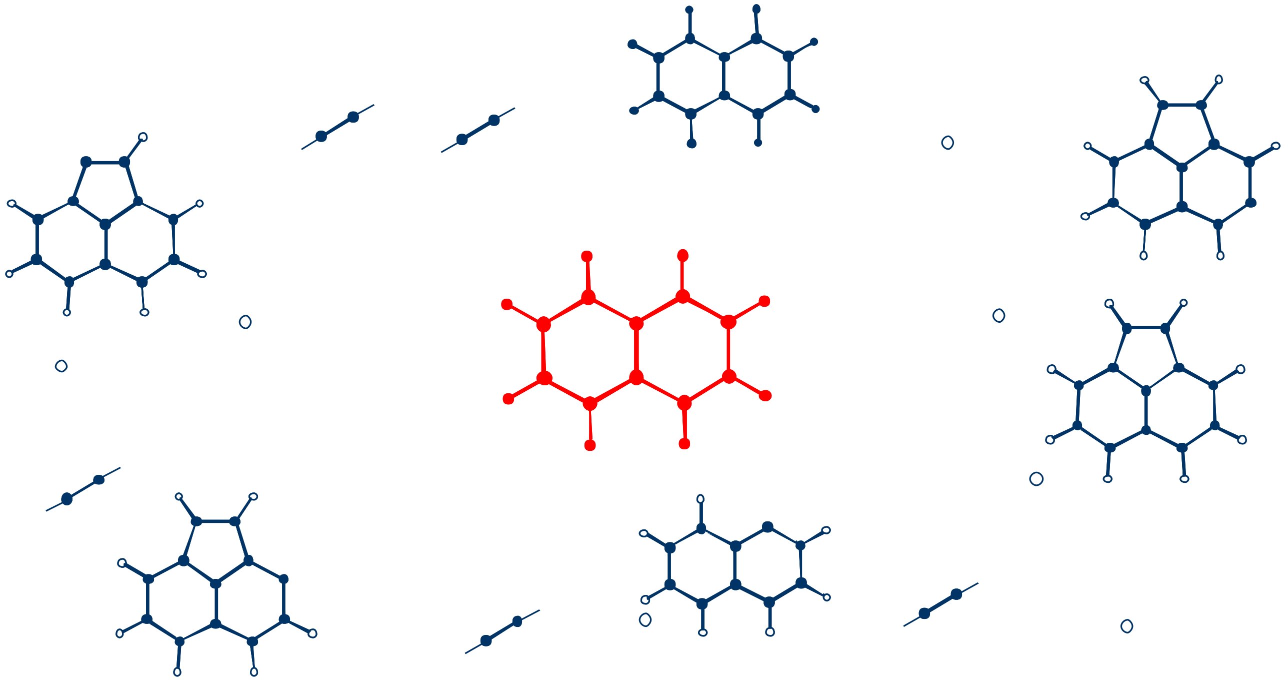


Particle zone

Molecular zone

Kinetic Monte-Carlo/Molecular Dynamics (KMC/MD) Simulations

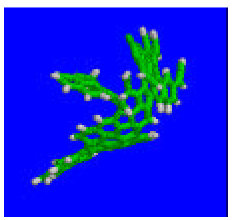
KMC/MD can be used to simulate soot particle inception
(Violi, Kubota, Pitz, Westbrook, Sarofim, 2002)

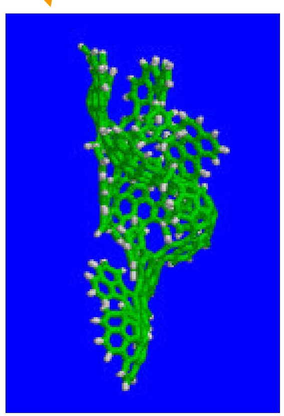


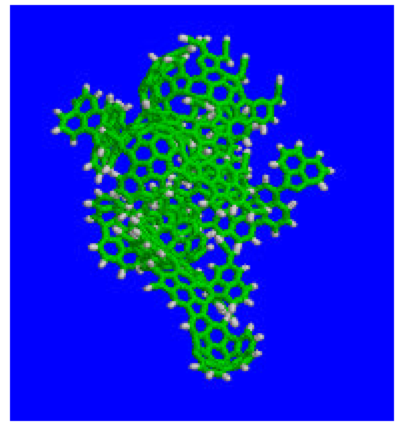
Inputs:

- Select initial species in gas-phase (above) and list of possible reactions

KMC/MD Simulations of PAH Growth and Particle Inception

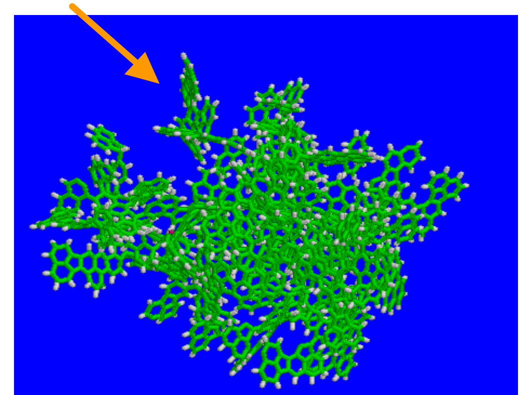






Images of computed PAH growth at various time steps.

Growth is due to:
-H abstraction
-Acetylene addition
-PAH polymerization



Kinetic Mechanism Development and Validation

Kinetic Mechanism Development

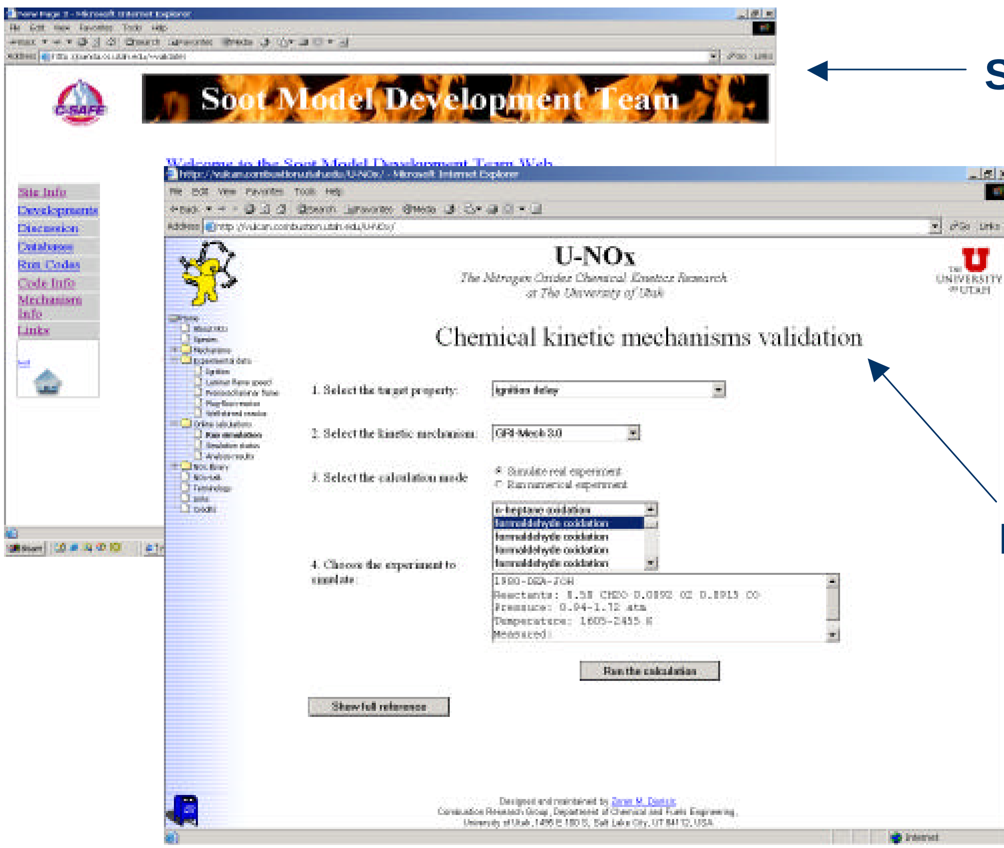
- Current efforts are focused on developing kinetic mechanisms for:
  - NO_x
  - High MW hydrocarbon fuels
  - Soot formation/oxidation
- Also development of web-based data repository and toolbox for kinetic analysis

Kinetic Mechanism Validation Web Site

- Repository for large number of digitized experimental data sets from literature
- Allows user to run simulations for experimental conditions of experimental data using different mechanisms
- Graphical comparison of simulation with data
- Various kinetic analysis tools for elucidating pathways

Kinetic Mechanism Validation Web Site

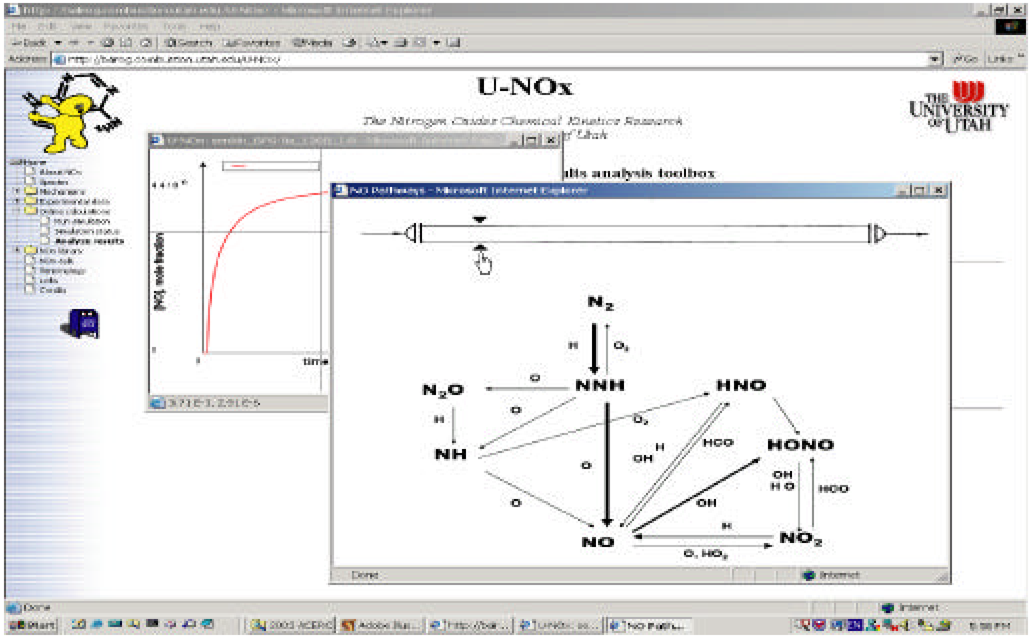
The Validation web site is a stand-alone tool that can be easily integrated into various chemistry-specific environments.



Soot kinetics research

NOx kinetics research

Reaction Pathway Analysis

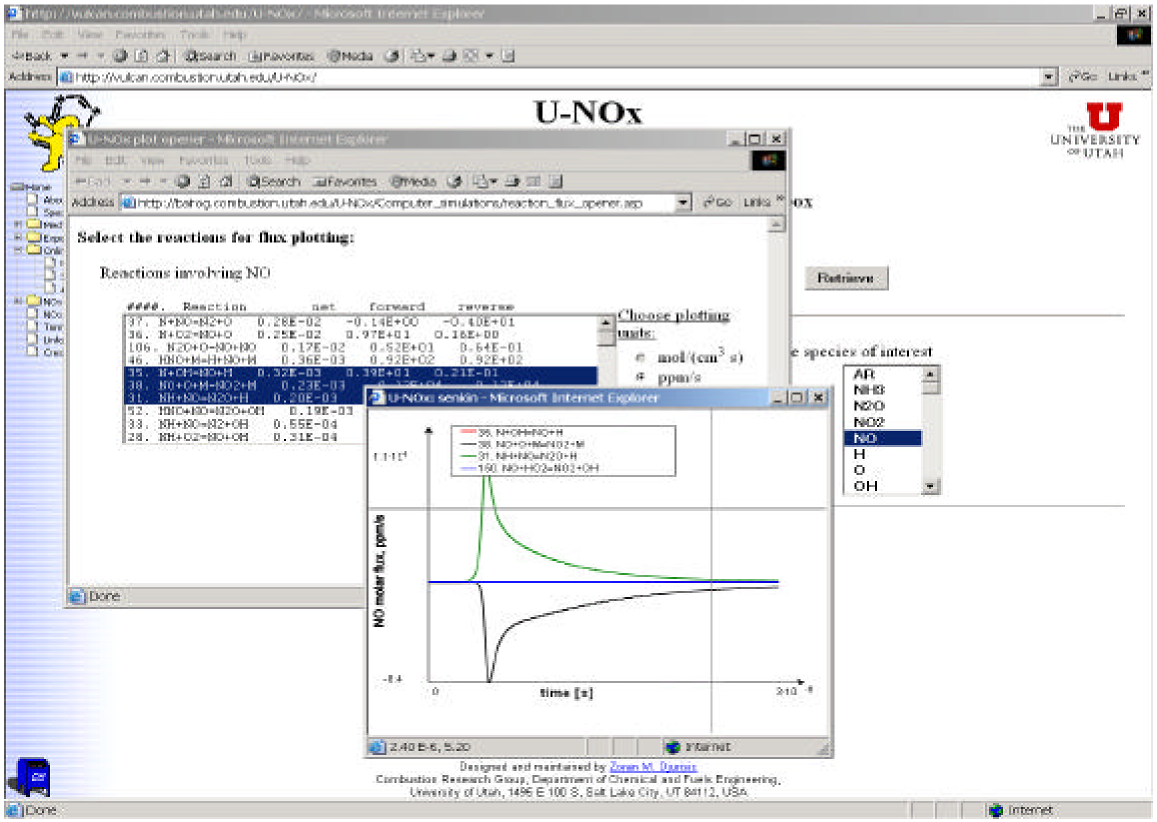


<u>Web-based tool allows:</u>

-Determination of rate-based reaction pathways at any point along reactor

-Relative magnitude of rates of intermediate paths indicated by thickness of connecting arrows

Species Flux Analysis



Web-based tool allows:

-Determination of flux of individual species throughout reactor due to a particular reaction

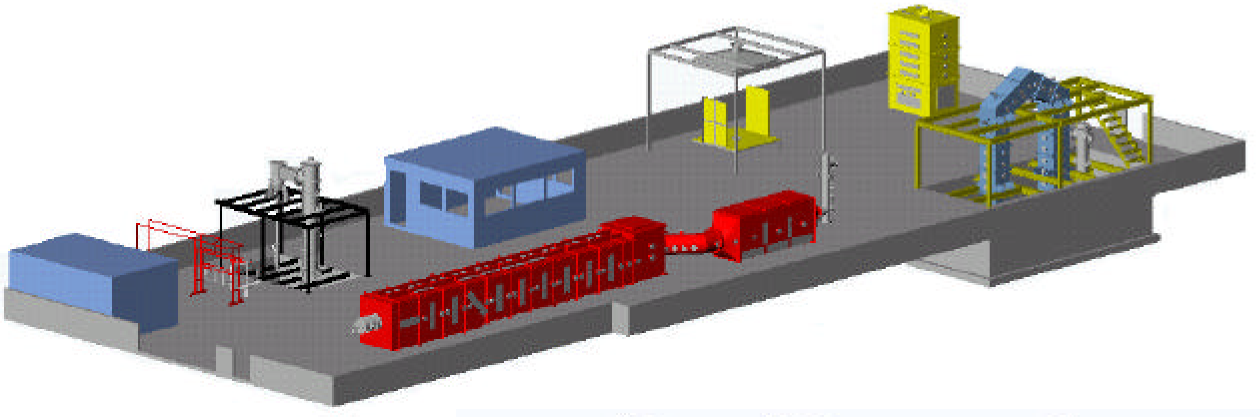
-Flux of a species due to multiple reactions can be plotted simultaneously

Process Development and Verification

Multi-Scale Testing Capabilities

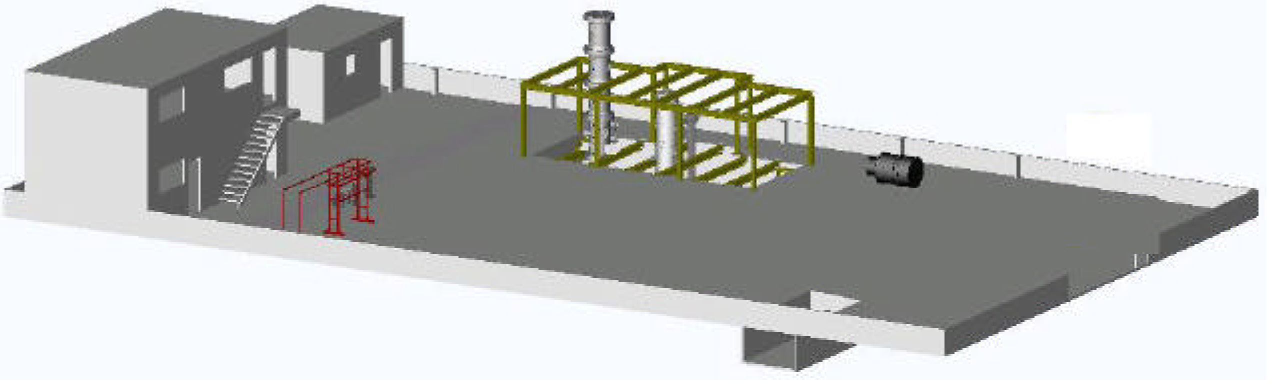
- Wide variety of bench- and pilot-scale combustion test facilities provide
  - Generation of model validation data at a credible scale
  - Scaled evaluation of process modifications, additions, sensors
  - Development and testing of pollution control technologies for a range of fuels and combustor types

Schematic of University of Utah Industrial Combustion & Gasification Research Facility



__Main Building Layout__

__Recent Expansion into Additional Building__



Located off-campus at 870 South 500 West
Salt Lake City, Utah

L1500 Test Facility

5 MMBtu/hr Pulverized Coal Test Furnace for study of:

-NOx control strategies

-Low NOx burners/staging

-Reburning

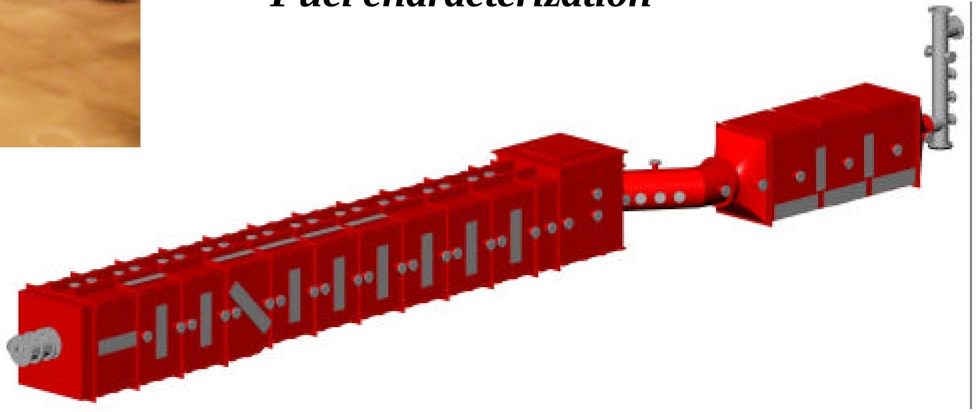
-SNCR/SCR

-Oxygen injection

-Corrosion/deposition

-Coal blends/cofiring

-Fuel characterization



Some Current/Recent Programs:

- NOx reduction via O_2 injection
- PRB/Ill#6 co-firing
- Biomass/biosludge co-firing

Pilot-Scale Stoker Facility

<u>1 MMBtu/hr grate-fired facility for study of:</u>

-Emissions from various fuels

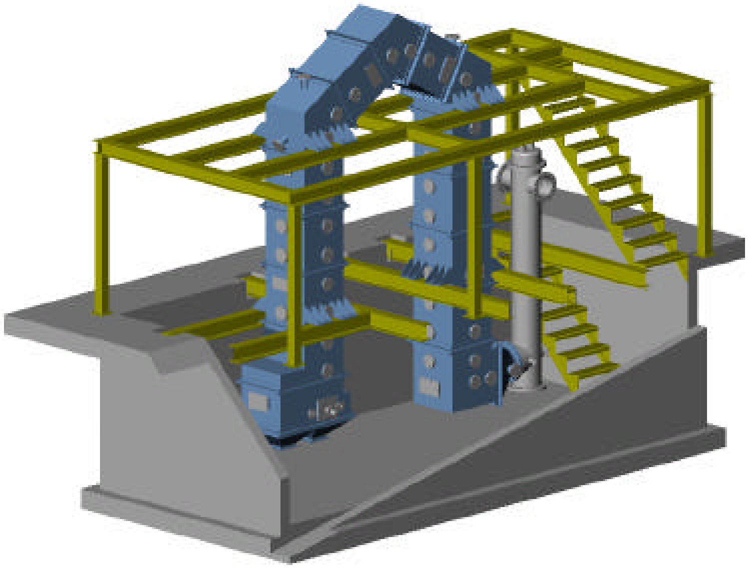
-Biomass, coal, tires, waste fuels

-Carbon loss

-NOx control strategies

-Corrosion/deposition

-OFA optimization

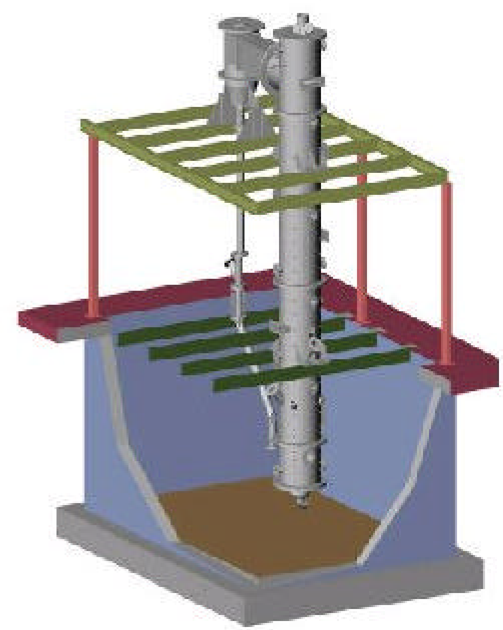


<u>Some Current/Recent Programs:</u>

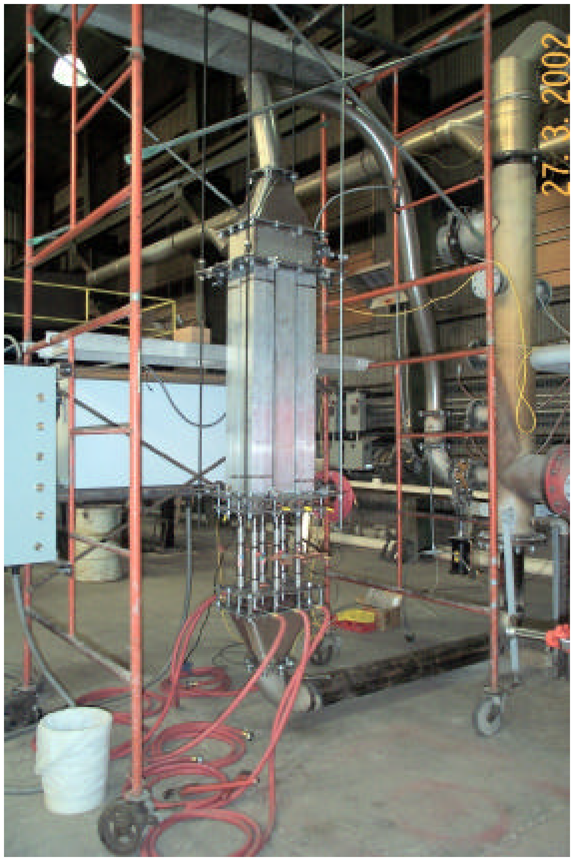
- emissions from wood firing
- coal/waste oil co-firing
- Biosludge co-firing

Pilot-Scale Circulating Fluidized Bed

1 MMBtu/hr fluidized-bed facility for study of:
-Bubbling or circulating operation
-Biomass, coal or waste fuels
-In-bed sulfur capture
-Emission control strategies



Field-Ready SCR Catalyst Slipstream Reactor

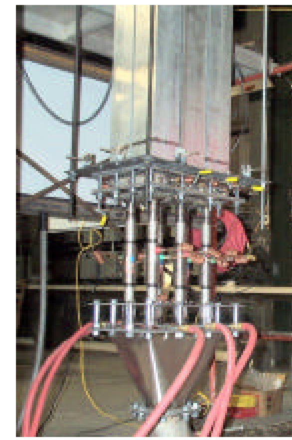


<u>SCR Catalyst Slipstream Reactor:</u>

- 6 separate catalyst chambers

- Independent pressure control and NOx measurement per chamber

- remote electronic control for operation and data acquisition

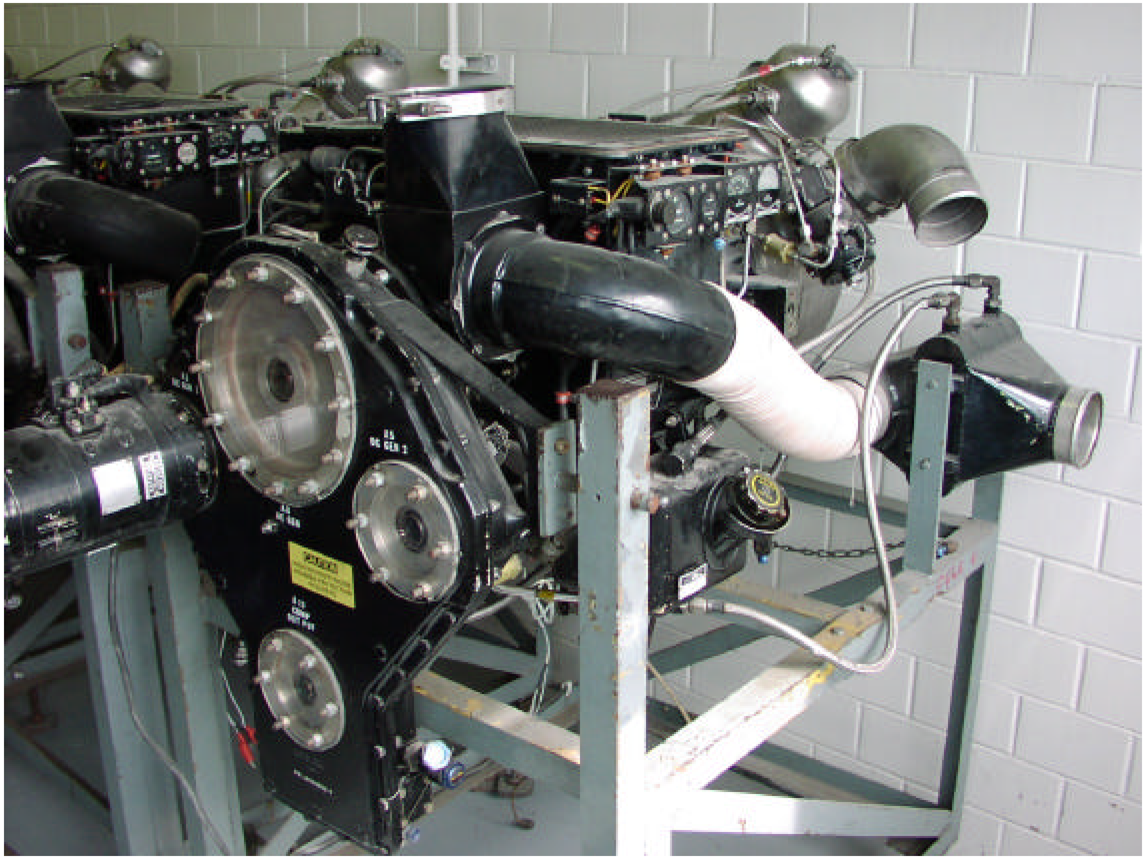


<u>Installations:</u>

- 6 month test in Rockport, IN (AEP)
  - PRB/E.Bituminous blend
  - tests of long-term catalyst deactivation and Hg Oxidation
  - begins mid-Oct. 2002
- 6 mo. test – site TBD
  - biomass/coal blend
  - catalyst deactivation

Team: REI, UofU, BYU, several catalyst vendors, utility participants – DOE funding

Gas Turbine Facility

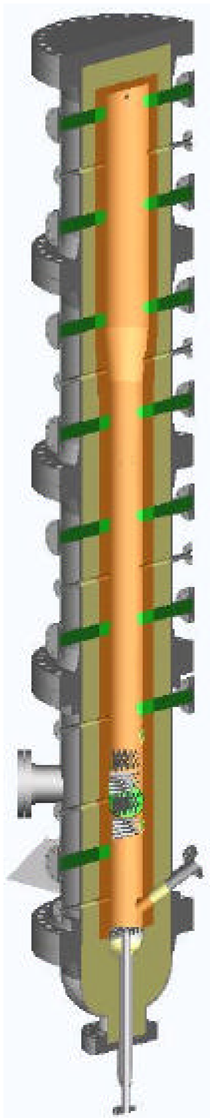


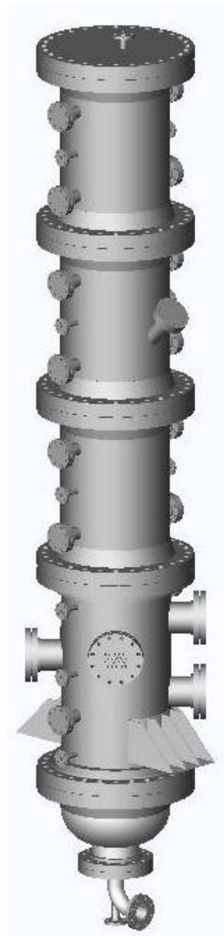
GTCP 85 Series Allied Signal Gas Turbine Engine

Aircraft Auxiliary Power Unit (APU) for study of:
-Particulate emissions
-NOx emissions

Current Programs:
- use of additives to reduce particulate emissions from jet fuel combustion (Jet-A/JP-8)

Fluidized Bed Gasifier



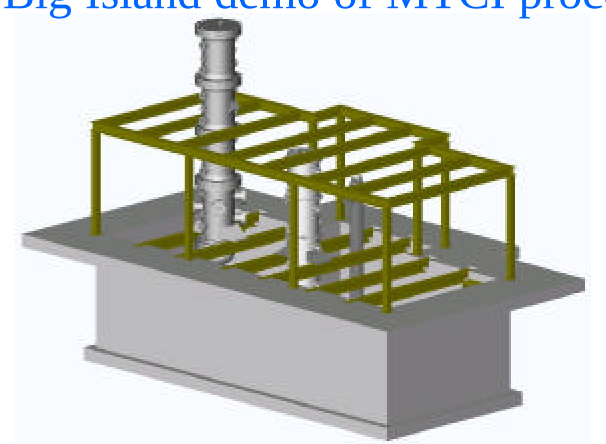


Pressurized Fluid-bed Steam Reformer for Black Liquor for study of:

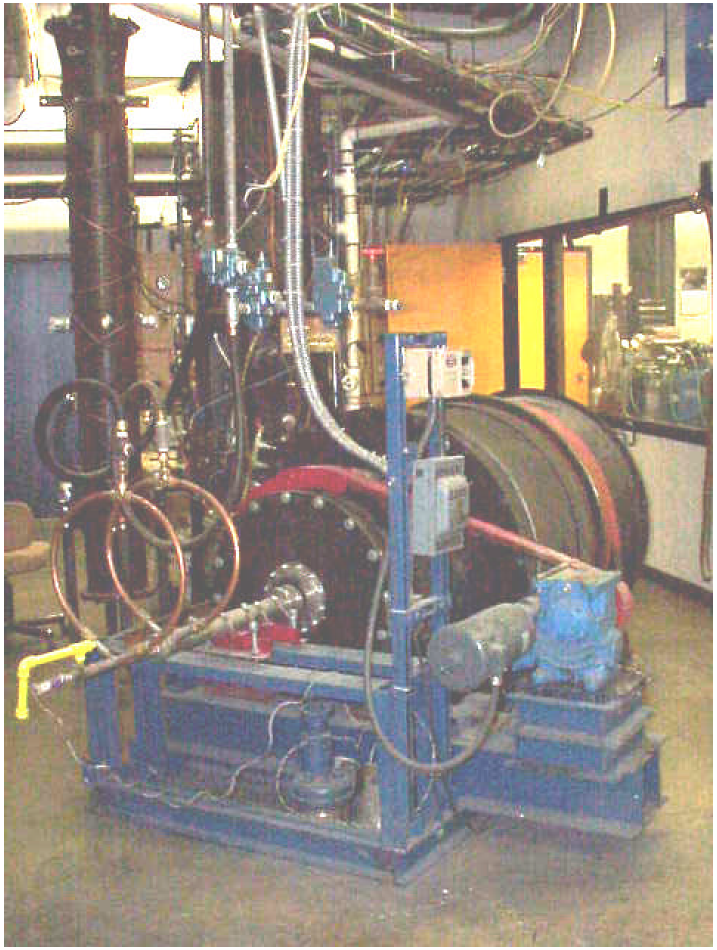
-Reaction chemistry
-Synthesis gas properties
-Bed agglomeration
-In-bed heat transfer

Current Programs:

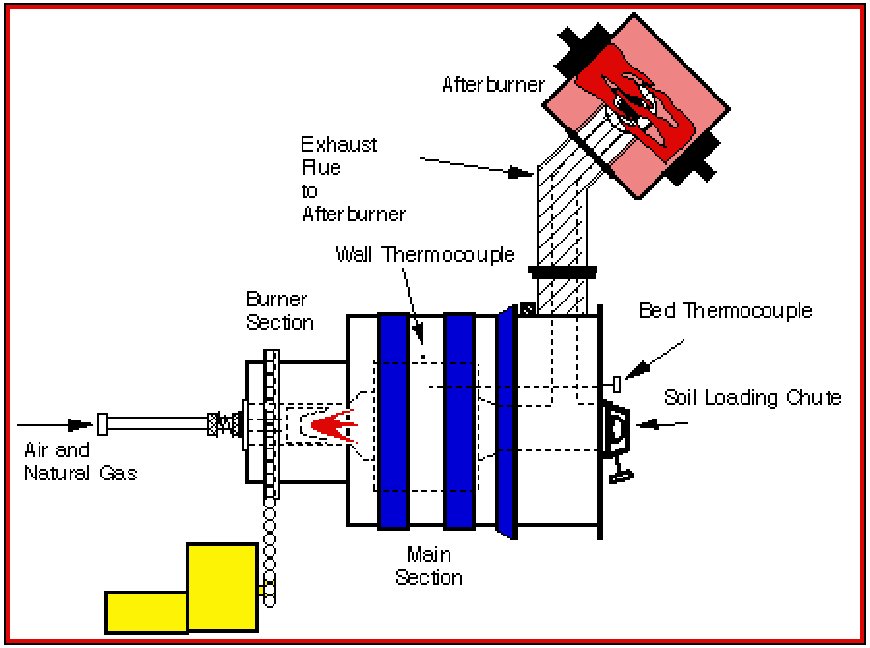
- DOE program in support of Georgia-Pacific Big Island demo of MTCI process



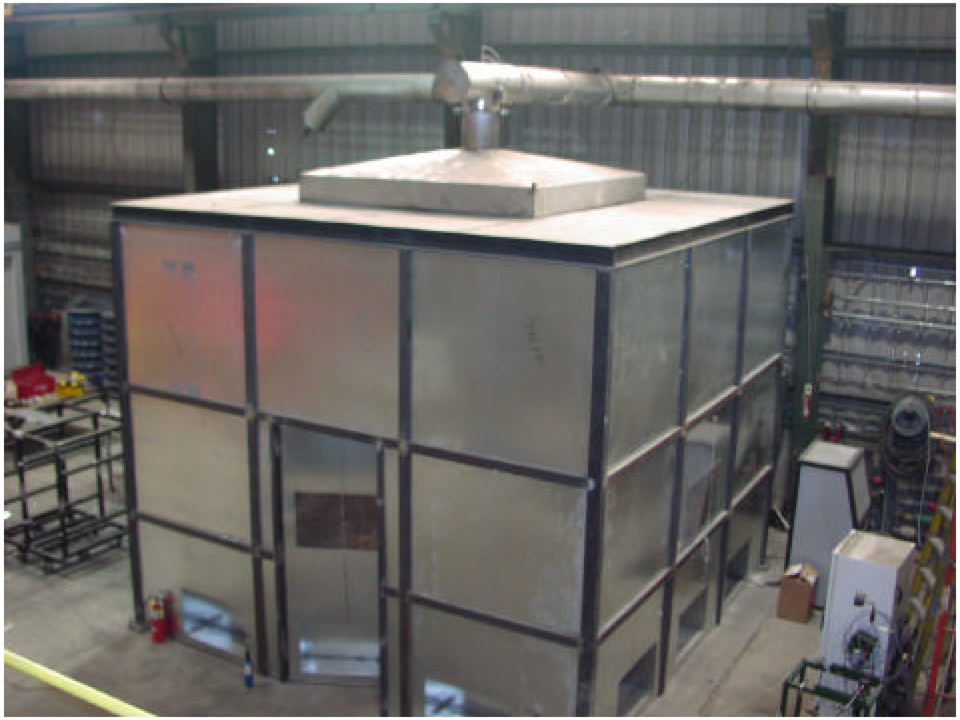
Pilot-Scale Rotary Kiln



0.5 MMBtu/hr Rotary kiln facility:
-Batch kiln simulate moving control volume
-2 ft. inner diameter
-0.35 MMBtu/hr afterburner tower
-Natural gas burner



Pilot-Scale Fire Test Facility



<u>Fire test facility for investigation of:</u>

-Jet fuel pool fires

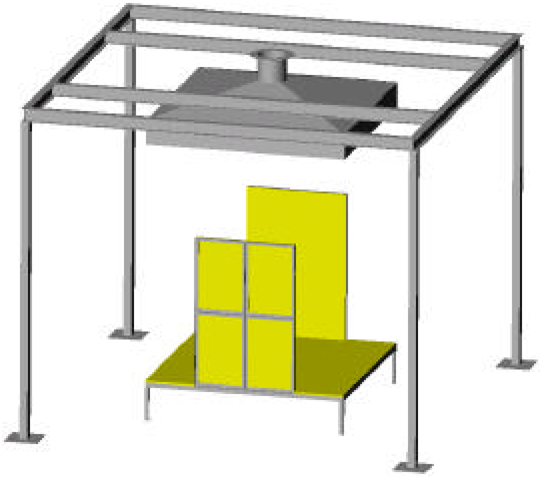
-Heat transfer

-Soot formation

-Surrogate fuel validation

-Wildfire fuel characterization

-Other fire scenarios



Remote-Site Sampling Capabilities

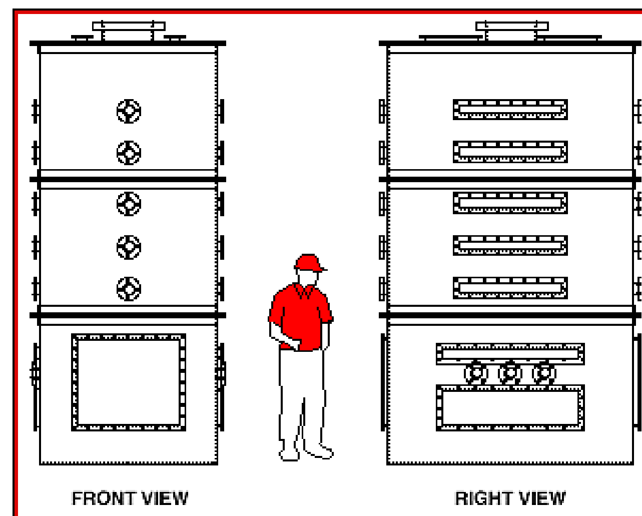
Mobile particle lab equipped with instrumentation for measurement of ultra fine and fine particulate:

-Scanning Mobility Particle Sizer (SMPS)
-Optical Particle Counter (OPC)
-Photoacoustic Analyzer (PA - for soot)
-Photoelectric Aersol Sensor (PAS)
-Miscellaneous particulate collection equipment

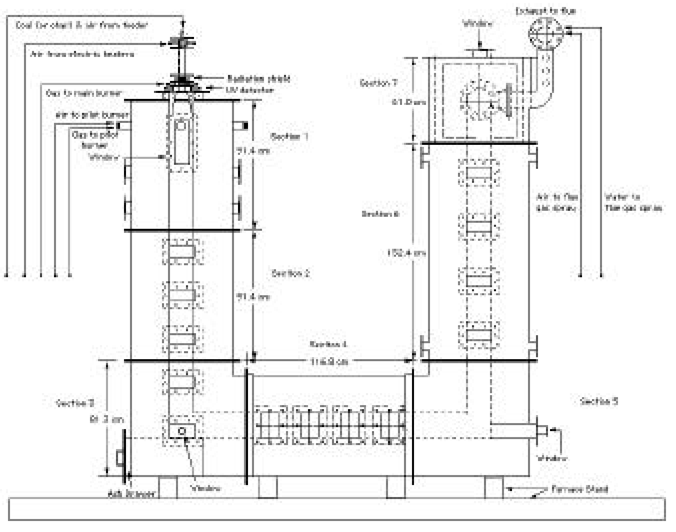
Brick Kiln/Process Heater

3 MMBtu/hr facility for simulation of:

-Process heater
-Brick kiln
-Reheat furnace
-Firing various fuels



Down-Fired Multi-Fuel Furnace



100,000 Btu/hr Pulverized Fuel facility:

-6 in. inner diameter

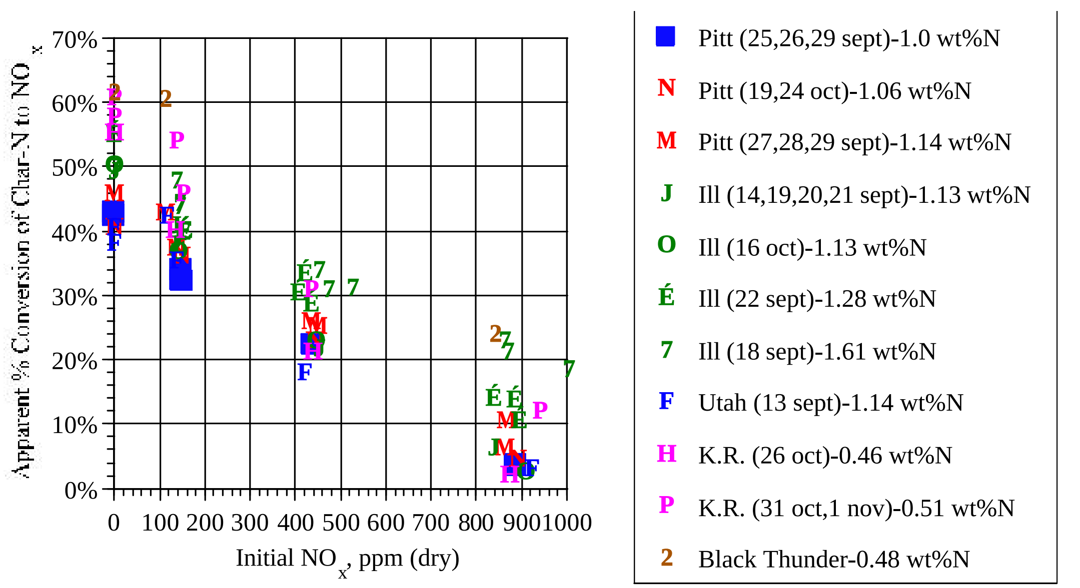
-axial or premixed burner

-Access ports for staging, reburning, SNCR

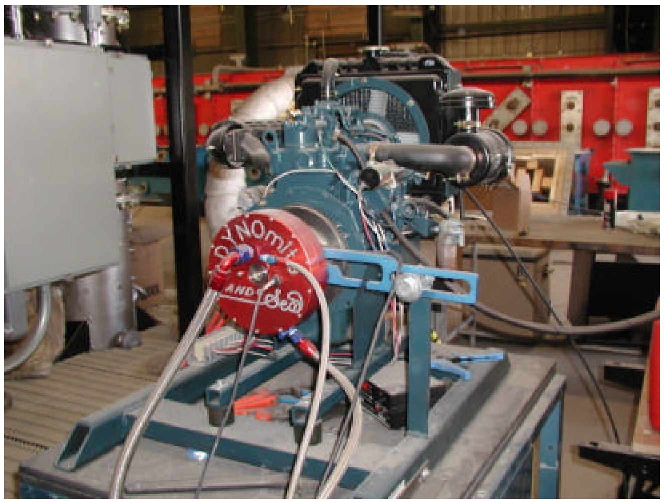
-Electric air preheat up to 800 F

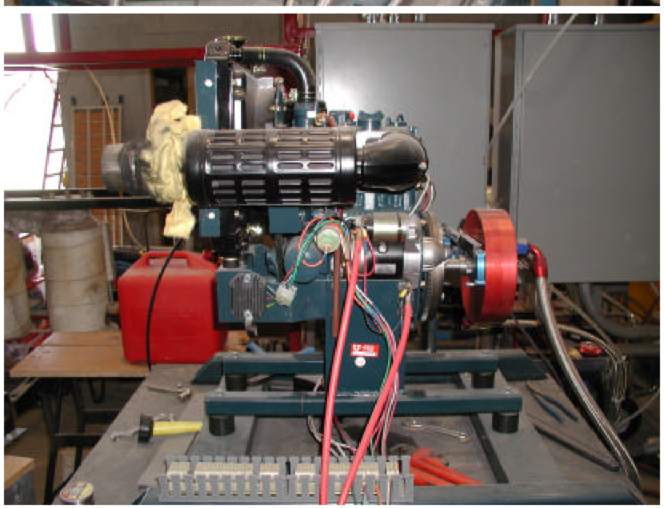
Some Current/Recent Programs:

- Hg speciation during coal firing
- Biosolids injection for NOx control
- Char N conversion to NO



Diesel Test Facility





<u>2 Cylinder Kubota Test Engine:</u>
-model Z482B, with 482 cc displacement
-water-break dynamometer with torque load control

<u>Some Current/Recent Programs:</u>

- fuel additives for particulate control
- chemical species fingerprints of diesel exhaust
- development of detailed chemistry for diesel soot formation
- sensor development/evaluation for diesel exhaust

Additional Test Facilities

Bench-Scale Fluidized Bed
- 6-inch I.D.
- electrically-heated
- solid/slurry feeding

Bench-Scale Rotary Kiln
- solids heating up to 30 K/min
- walls heated by 25 kW induction heating system
- variable rpm

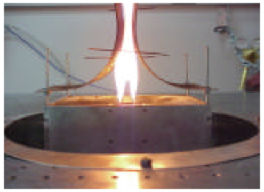
Process Simulation

Computational Combustion

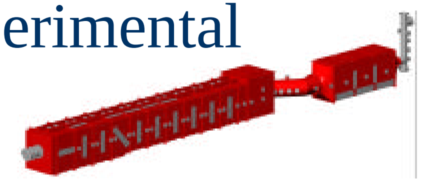
- Development of Computational Fluid Dynamics based simulation tools for
  - Large-scale fires
  - Various industrial furnaces including
    - Coal-, oil- and gas-fired boilers
    - Incinerators, kilns, process heaters, flares
- Tools useful for simulating full-scale industrial equipment and scaling up intermediate results
- Close working relationship with CFD services company
  - Reaction Engineering International

Technical Approach

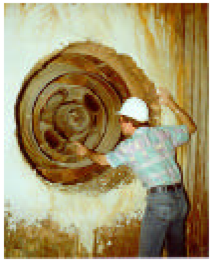
- Use experimental capabilities to study controlling mechanisms for various fuels
  - For pollutant emissions or key operational problems



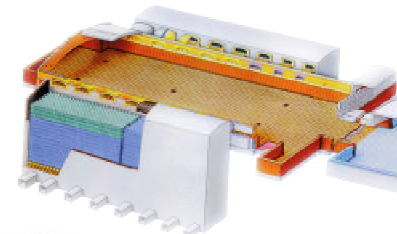
- Develop theoretical models describing controlling physics
- Incorporate models into combustion simulations
- Validate combustion models over range of experimental scales



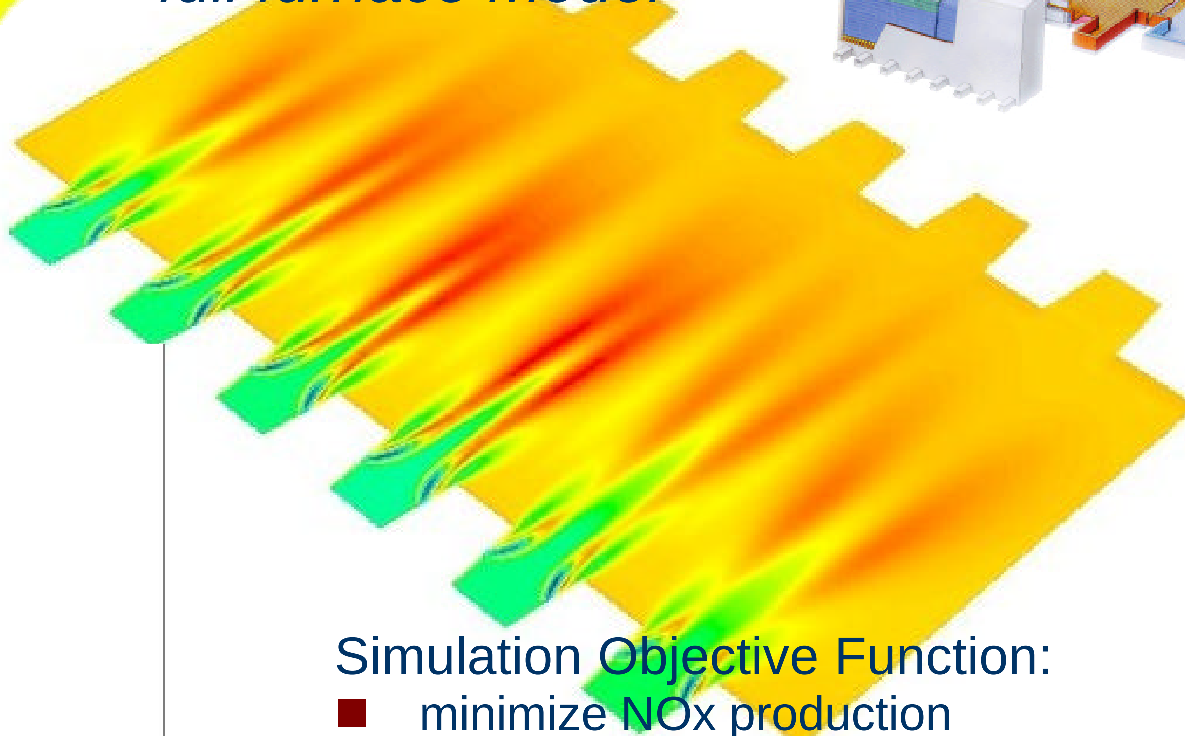
- Apply simulation tools to practical combustion systems



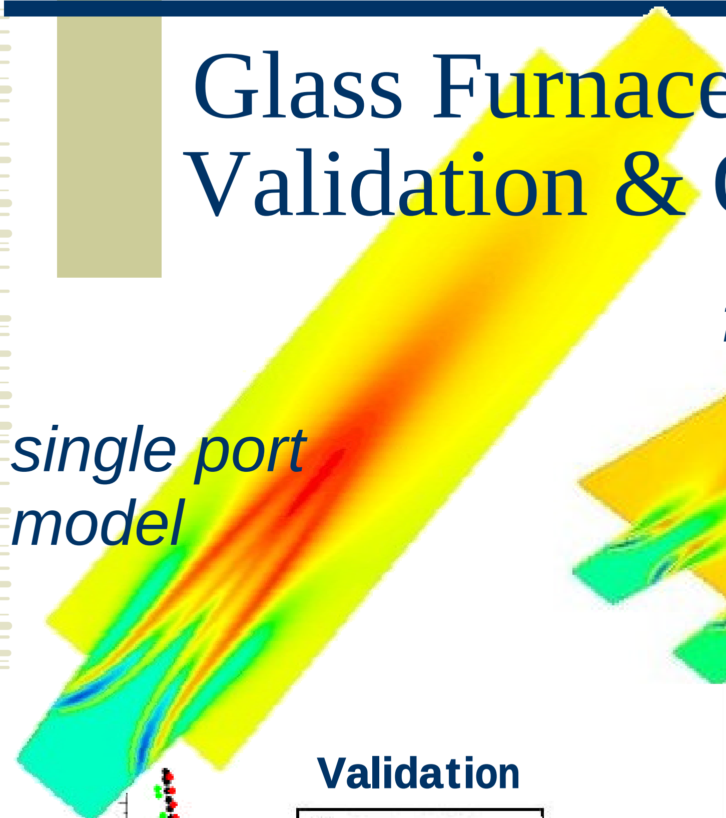
Glass Furnace Simulation, Validation & Optimization

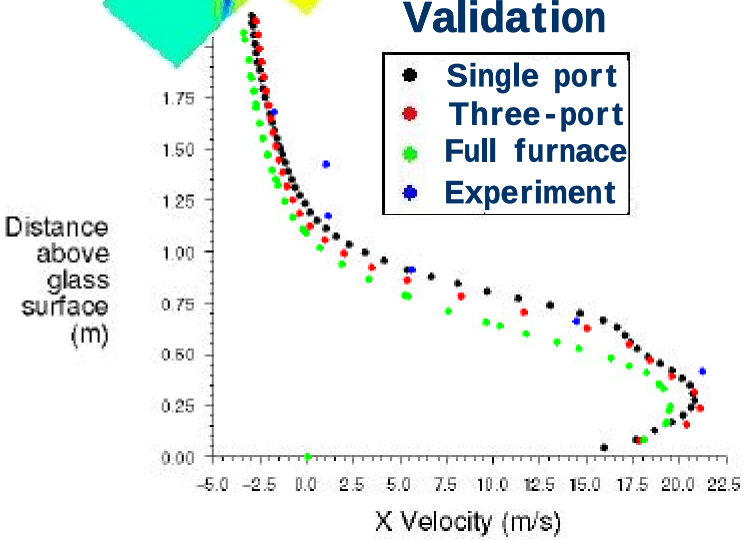


full furnace model



single port model





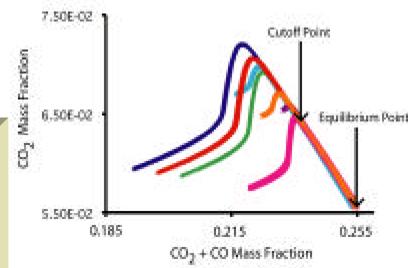
Simulation Objective Function:

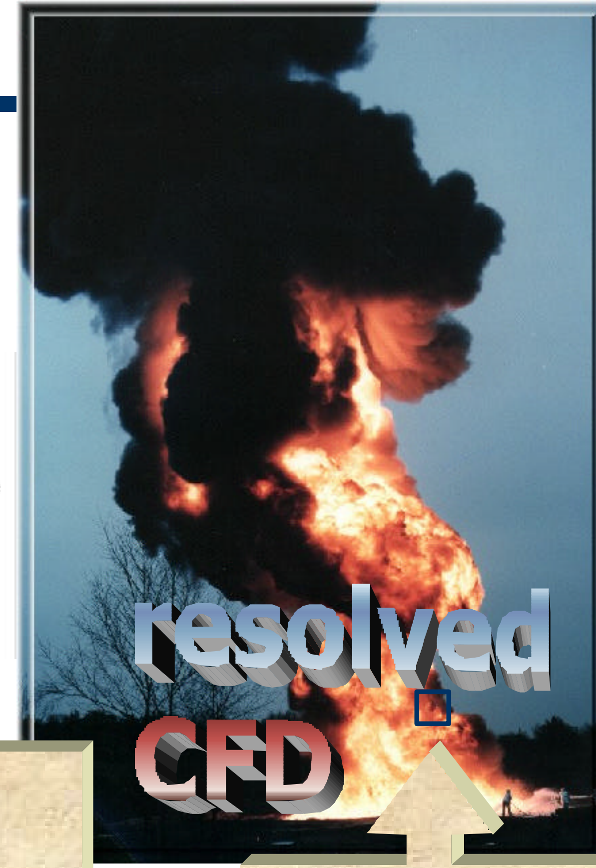
- minimize NOx production
- by adjusting manipulable operating variables
- subject to constraint of maintaining heat flux profile to glass melt.

Challenges for Computational Combustion

- Need to incorporate relevant fundamental mechanistic information into simulations
  - Temporal and spatial scales of physical/chemical processes involved may span many orders of magnitude
  - Computer limitations limit level of resolution
  - Many key processes occur below resolved scale and thus requires development of accurate “sub-grid” models
    - Often involves novel mathematical techniques as well as engineering approximations
- Perform verification of coding and validation of accuracy of the simulation
  - Demonstrate ability for scale-up utilizing laboratory data at multiple spatial scales
  - Demonstrate ability to reproduce key physical observables and typical operating trends at full-scale

Sub Grid Scale Models





Molecular Scale
Elementary Chemical Kinetic Mechanism

100's of rxns
1000's of species

Mechanism Reduction

100's of species

validation
chem. kinetic mech.

Reaction Model

continuum micro
-reduce degrees of freedom
(resolved field vars)
-molecular scale transport
-radiation props.

Mixing Model

mesoscale model
(subgrid hetero. due to turbulence)
-nonlinear
-filtering/ averaging